# Optimization of the binding properties of a synthetic anion receptor using rational and combinatorial strategies

Kubik, Stefan; Goddard, Richard; Otto, Sijbren; Pohl, Susanne; Reyheller, Carsten; Stüwe, Sabine

*Published in:*
Biosensors and Bioelectronics

*DOI:*
10.1016/j.bios.2004.01.035



*Publication date:*
2005

*Biosensors Bioelectronics.*

# Optimization of the binding properties of a synthetic anion receptor using rational and combinatorial strategies

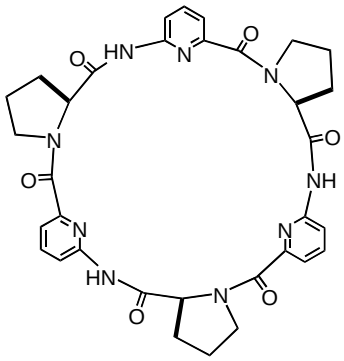
Stefan Kubik[a],[*] Richard Goddard[b], Sijbren Otto[c], Susanne Pohl[a], Carsten Reyheller[a], Sabine Stüwe[a]

[a] *Institut für Organische Chemie und Makromolekulare Chemie, Heinrich-Heine-Universität, Universitätsstr. 1, D-40225 Düsseldorf, Germany, Email: kubik@uni-duesseldorf.de*

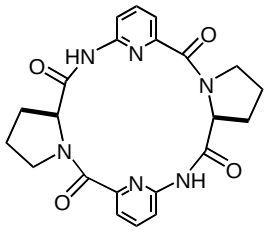
[b] *Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, D-45470 Mülheim/Ruhr, Germany*

[c] *Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, U.K.*

Structure of compounds **2** and **3**:

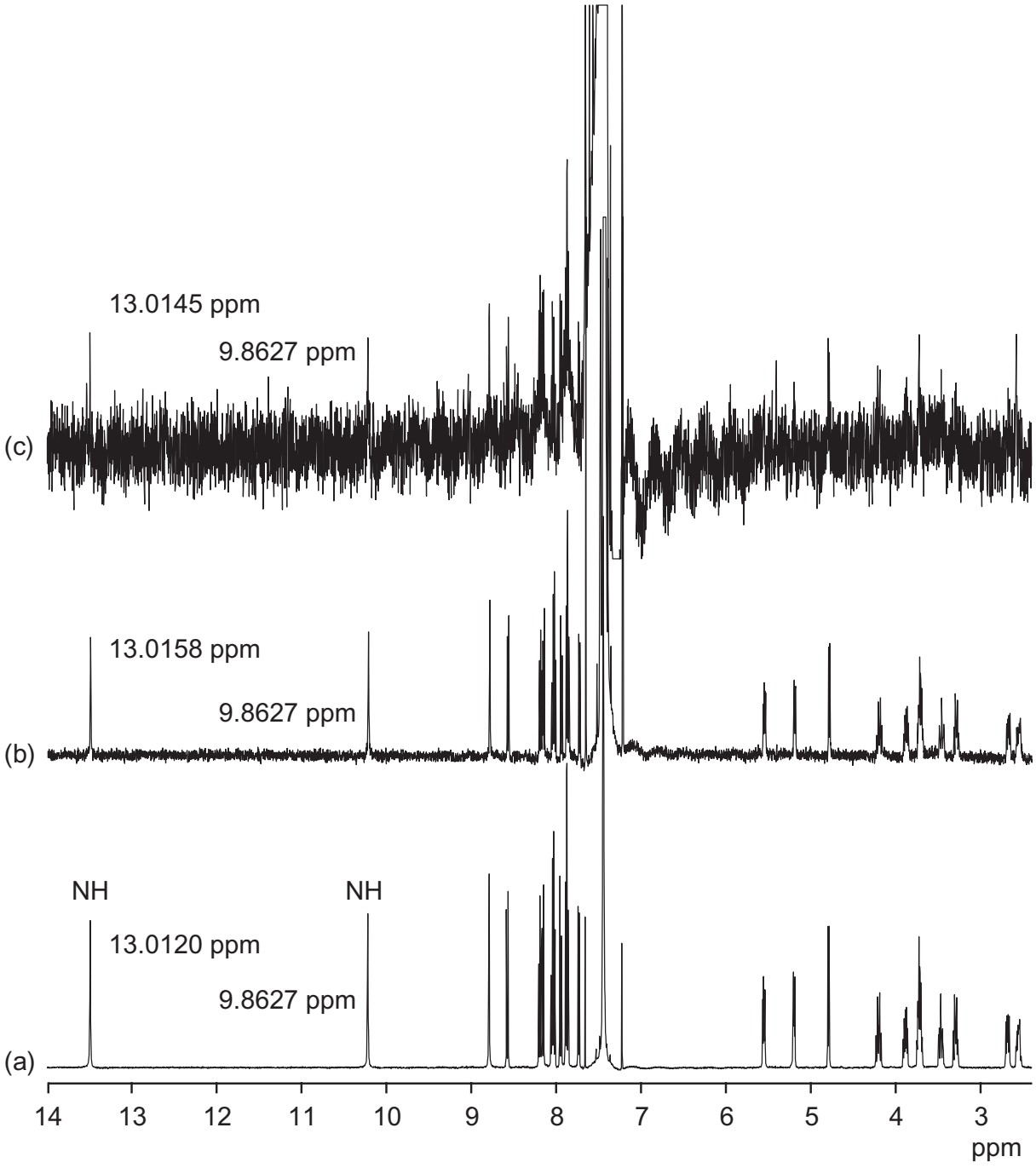


**2**

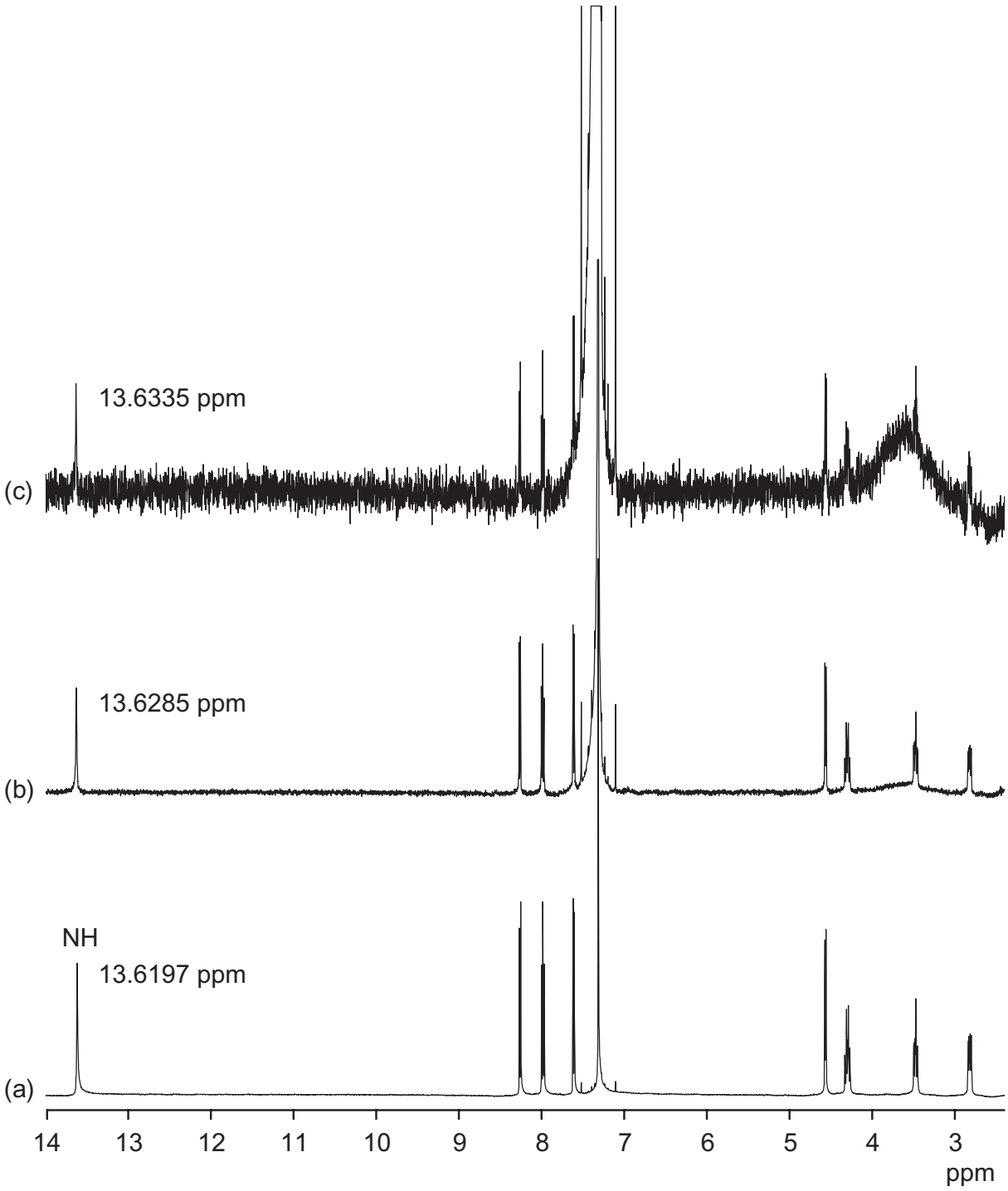


**3**

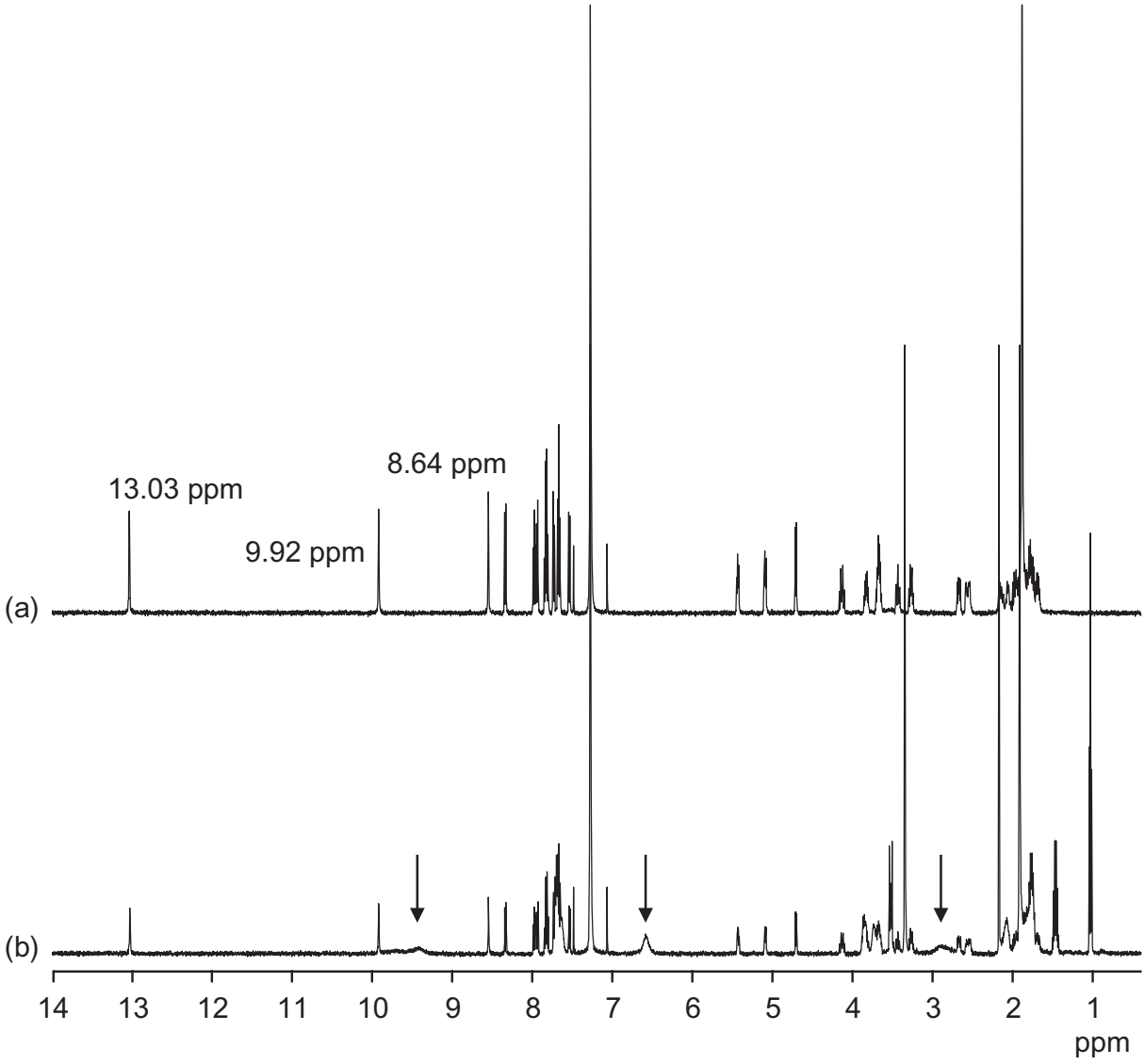
Concentration-dependent NMR spectra: **2** in $CDCl_3$ (a) 2 mM, (b) 0.2 mM, (c) 0.02 mM (Bruker DRX 500 / 500 MHz)



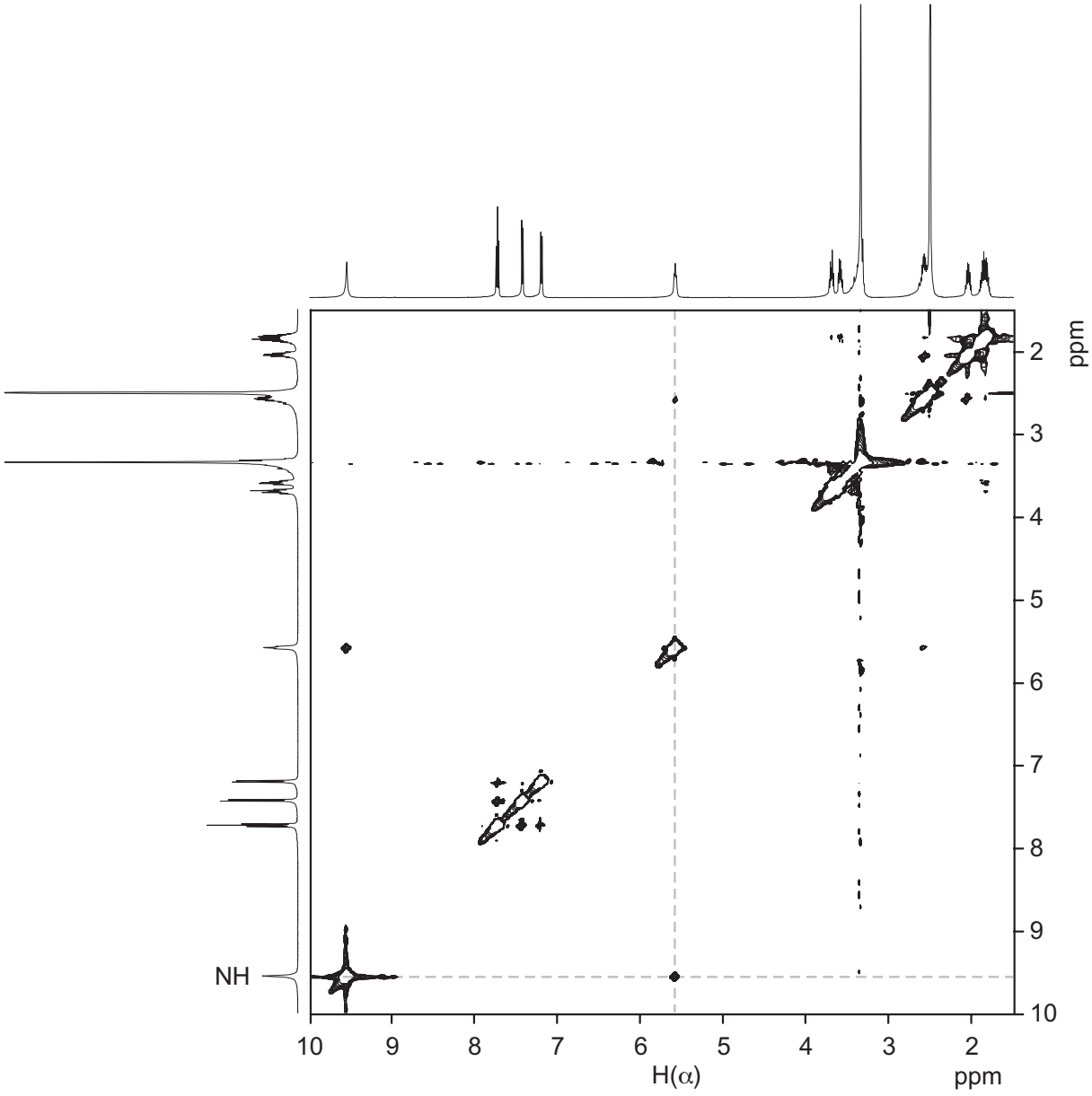
Concentration-dependent NMR spectra: **3** in $CDCl_3$ (a) 2 mM, (b) 0.2 mM, (c) 0.02 mM (Bruker DRX 500 / 500 MHz)



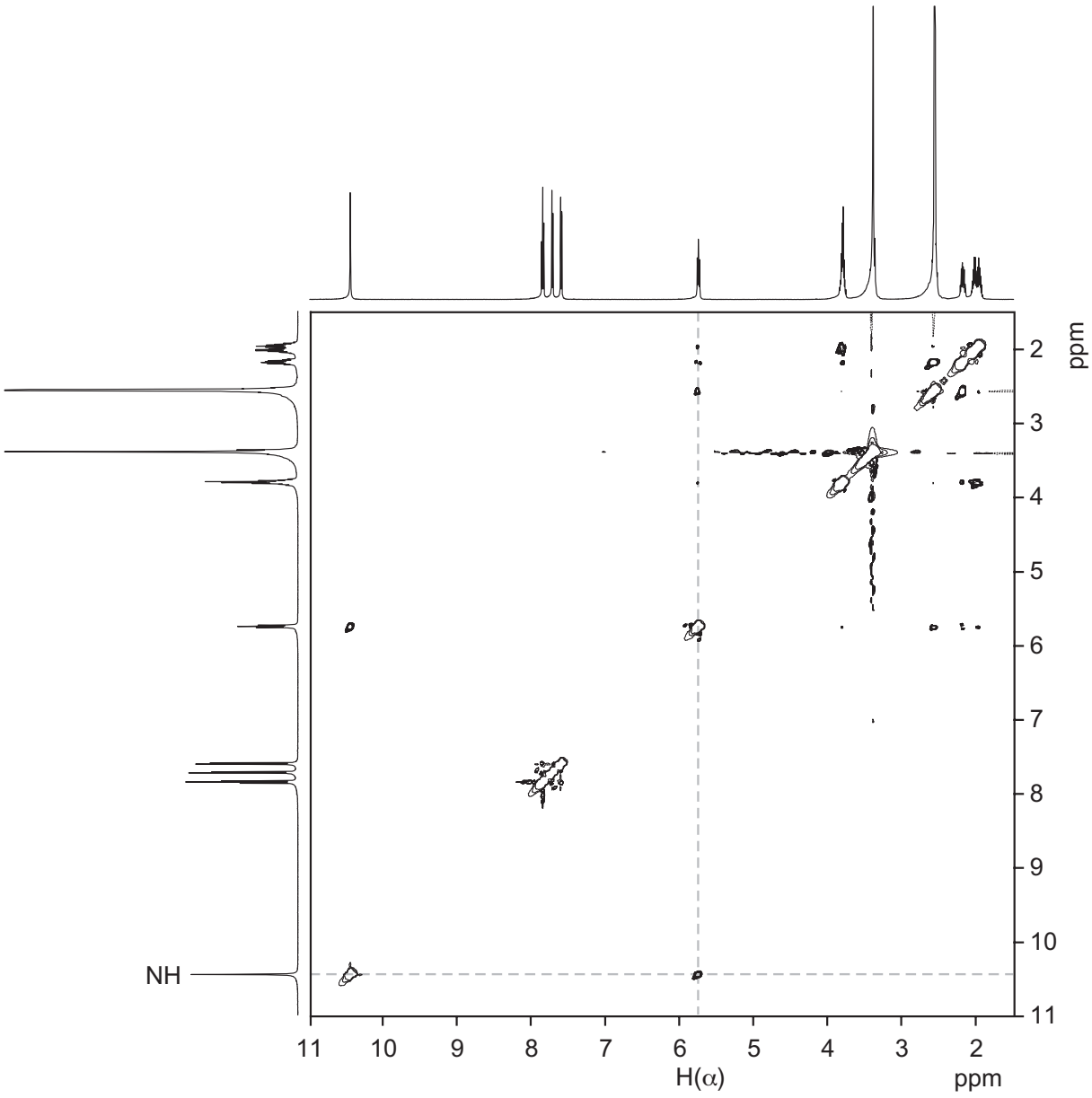
$^{1}$H-NMR spectra: **2** (1 mM) in $CDCl_3$ (a), **2** (1 mM) + 1 equiv of *n*-butyltrimethylammonium iodide in $CDCl_3$ (b).



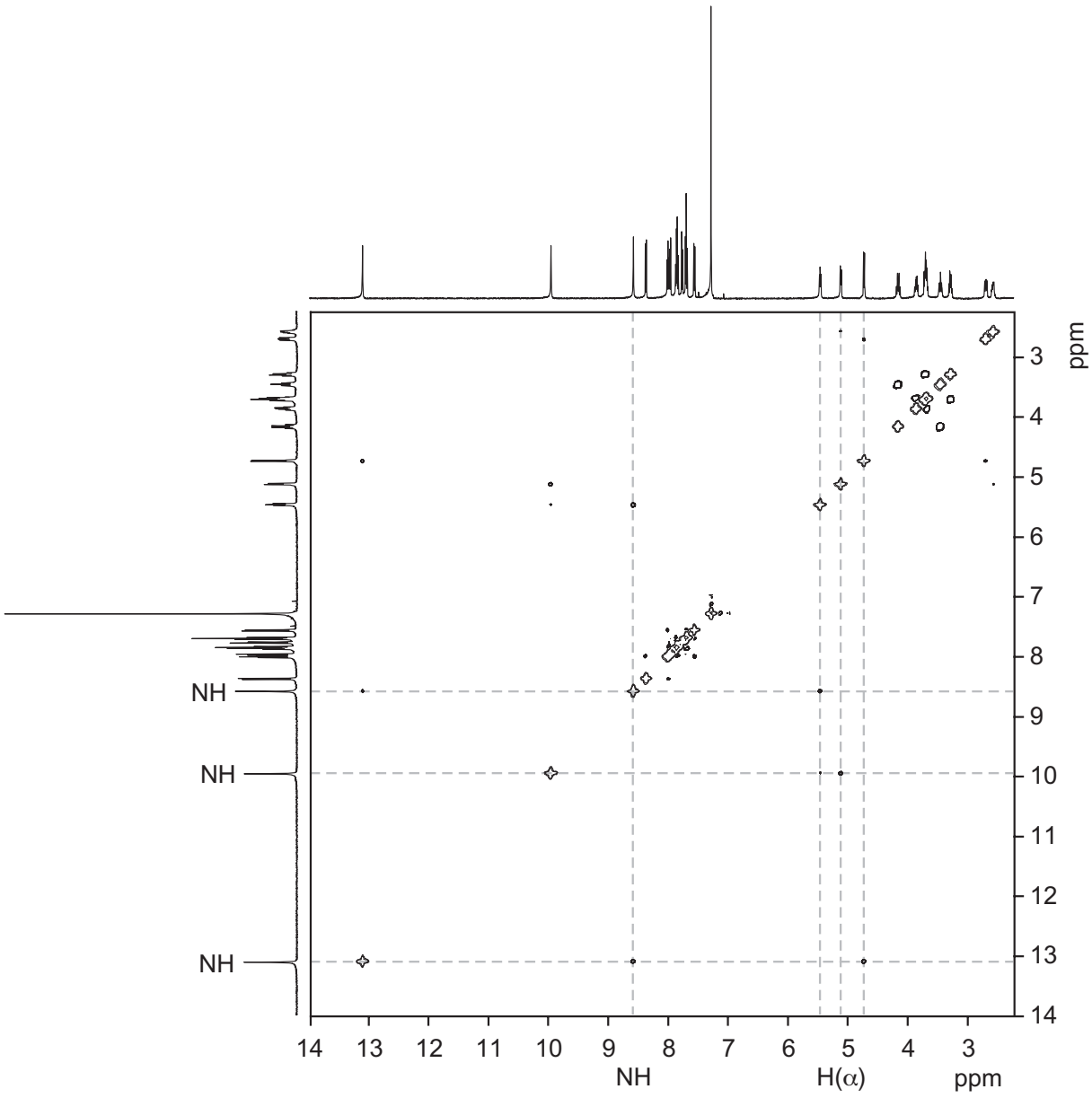
NOESY NMR spectrum: **2** (1 mM) in $d_6$-DMSO (mixing time 300 ms) (Bruker DRX 500 / 500 MHz).



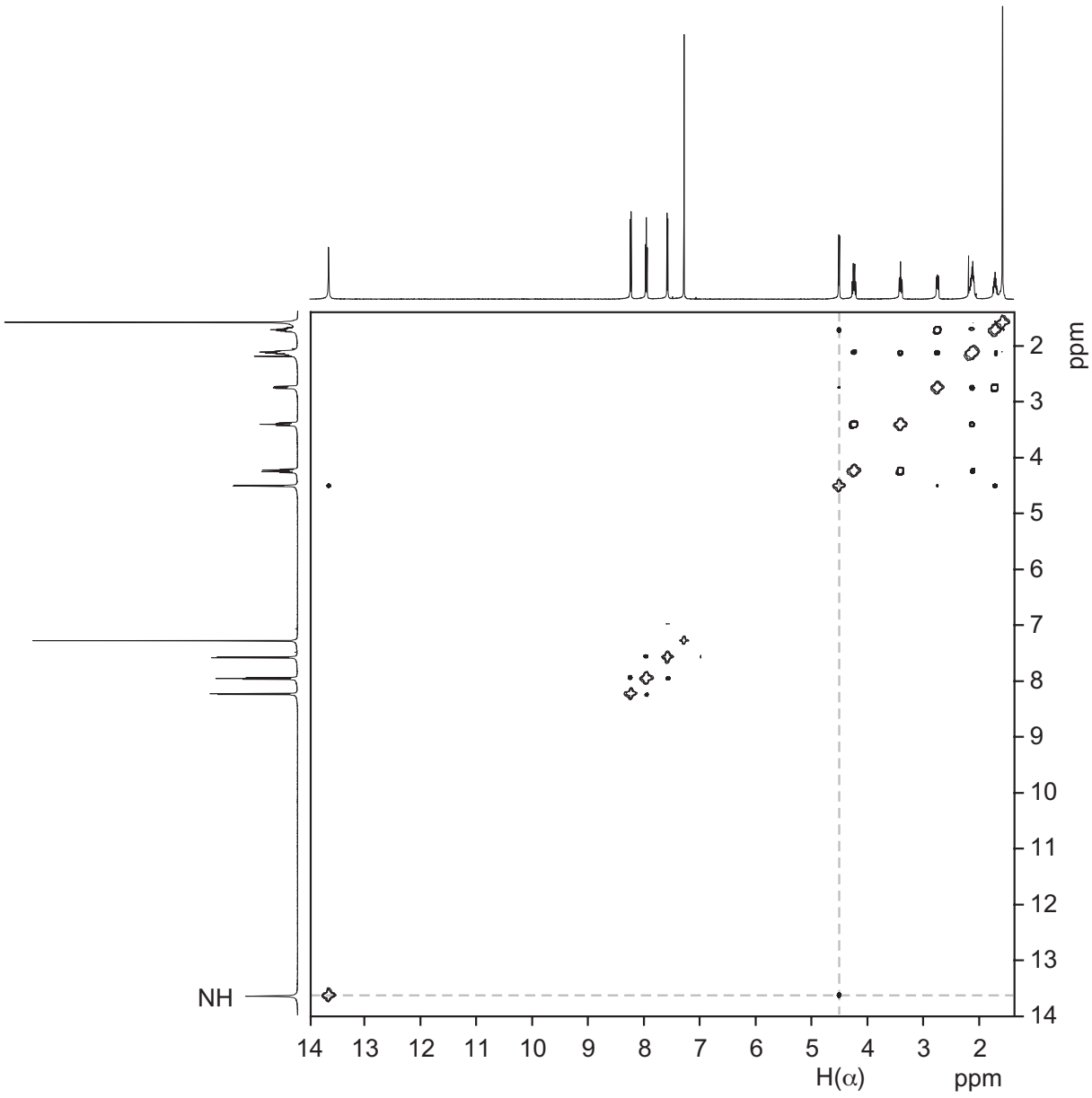
NOESY NMR spectrum: **3** (1 mM) in $d_6$-DMSO (mixing time 300 ms) (Bruker DRX 500 / 500 MHz).



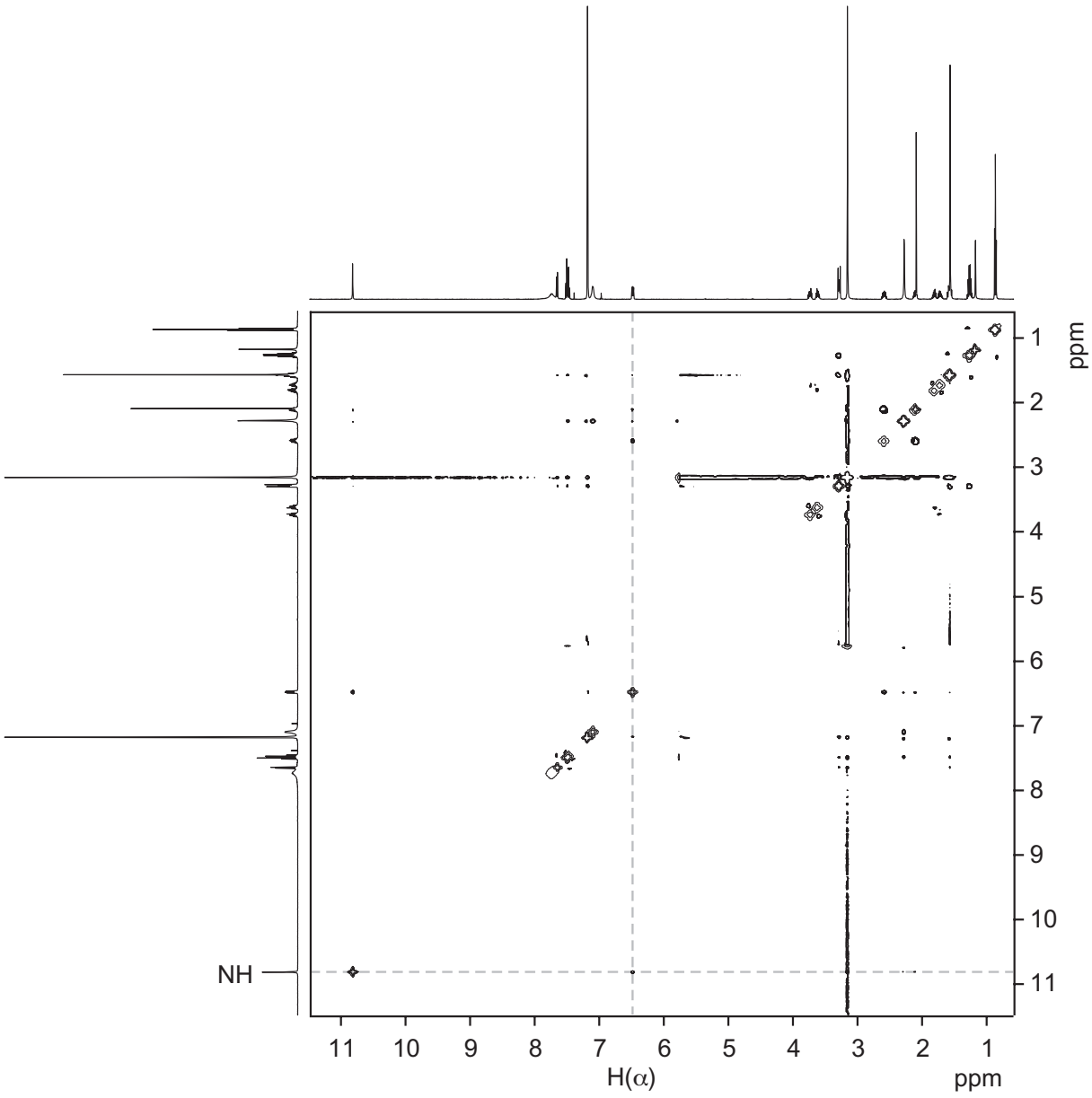
NOESY NMR spectrum: **2** (1 mM) in $CDCl_3$ (mixing time 300 ms) (Bruker DRX 500 / 500 MHz).



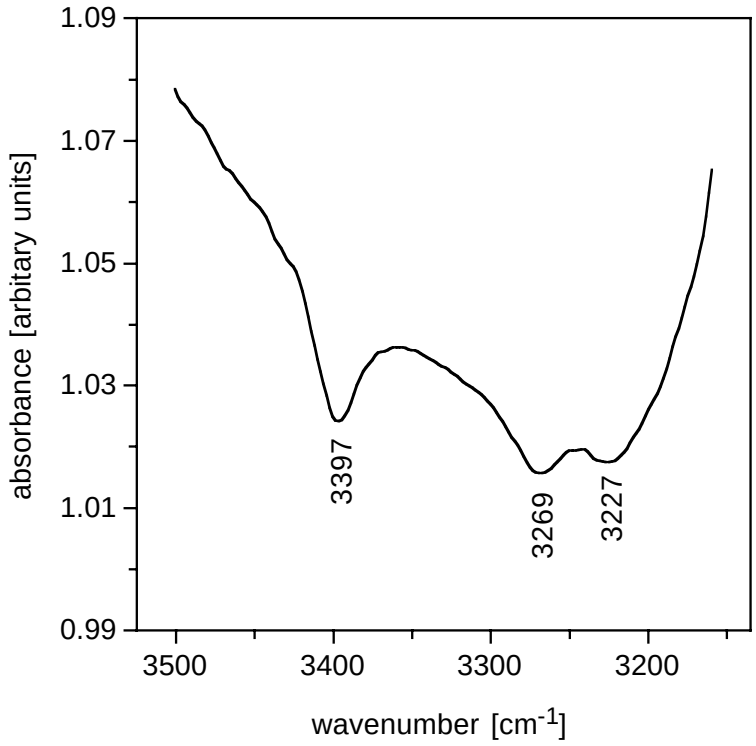
NOESY NMR spectrum: **3** (1 mM) in $CDCl_3$ (mixing time 300 ms) (Bruker DRX 500 / 500 MHz).



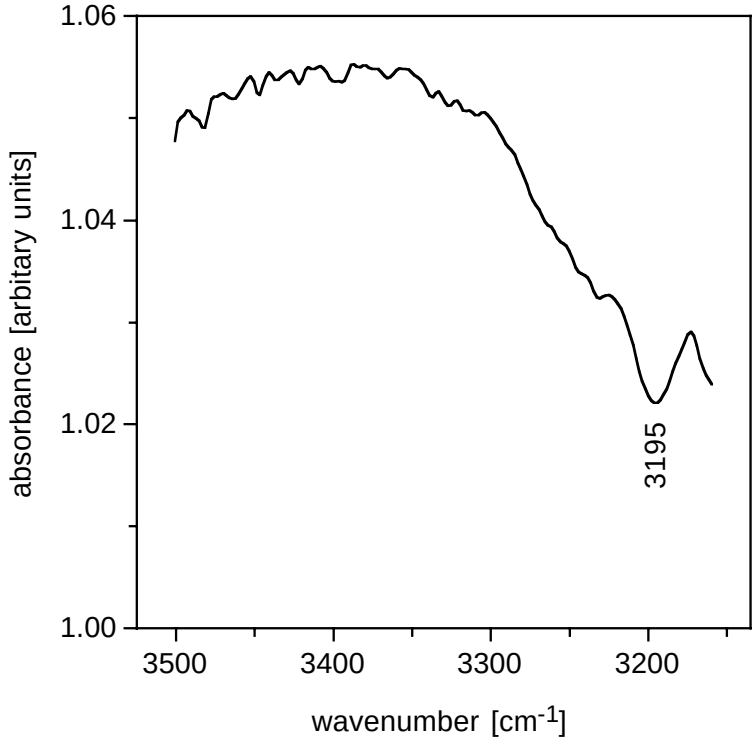
NOESY NMR spectrum: **2** (1 mM) after the addition of 3 equiv. of *n*-butyltrimethylammonium tosylate in $CDCl_3$ (mixing time 300 ms) (Bruker DRX 500 / 500 MHz).



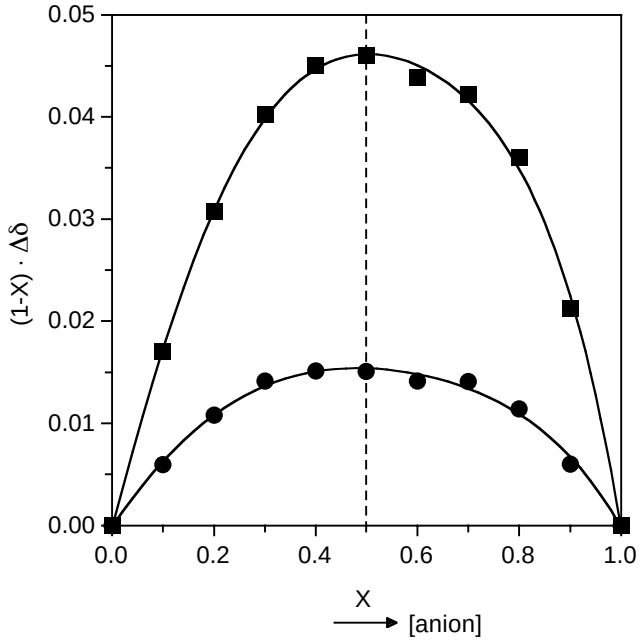
FT-IR spectrum: **2** in 1% [$d_6$]DMSO/$CDCl_3$ (c = 2mM)




FT-IR spectrum: **3** in $CDCl_3$ (c = 2mM)



Job-Plot: **2** + *n*-butyltrimethylammonium iodide in $d_6$-DMSO (Δδ = variation of the shift of the ProH(α) (squares) and the APAH(3) signal (circles) of **2**).




NMR Titration: Experimental (circles, squares) and calculated (line) saturation curves for the complex formation between **2** and *n*-butyltrimethylammonium iodide in $d_6$-DMSO (Δδ = variation of the shift of the ProH(α) (squares) and the APAH(3) signal (circles) of **2**)